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We discuss some of the the research that has been carried out with the support of grant number AFOSR-88-0197. The topics discussed are the numerical simulation of viscous incompressible flows, the numerical approximation of certain control problems, the analysis and application of centroidal Voronoi grids, and a book on finite element methods for viscous incompressible flows. For the sake of brevity, we will not go into great detail in the following discussion; further information concerning these topics can be gained from the appropriate references listed at the end of this section.

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FINAL TECHNICAL REPORT FOR GRANT NUMBER AFOSR-88-0197
TO CARNEGIE MELLON UNIVERSITY

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We discuss some of the the research that has been carried out with the support of grant number AFOSR-88-0197. The topics discussed are the numerical simulation of viscous incompressible flows, the numerical approximation of certain control problems, the analysis and application of centroidal Voronoi grids, and a book on finite element methods for viscous incompressible flows. For the sake of brevity, we will not go into great detail in the following discussion; further information concerning these topics can be gained from the appropriate references listed at the end of this section.

1 - Numerical Simulation of Viscous Incompressible Flows

a - Continuation methods

Typically, the nonlinear equations resulting from discretizations of the Navier-Stokes equations are solved via an iterative method such as Newton's method or a quasi-Newton method. For interesting values of the Reynolds number, these iterative methods converge only when a sufficiently good initial guess is available. A popular class of methods for generating good initial guesses are continuation methods wherein information obtained at lower values of the Reynolds number is used to determine the initial guess. In order to define a continuation method one must select a step size in the Reynolds number and then choose a prediction algorithm that, using previously obtained information, determines the initial guess.

Our research has shown that due to the nature of solutions of the Navier-Stokes equations it essentially doesn't matter which prediction algorithm is employed. For example, one can take the same step size in the Reynolds number whether one simply sets the inital guess to be the solution at a lower value of the Reynolds number or if one uses a more complicated tangent plane approximation to generate the initial guess. Furthermore, we have shown that the allowable step in the Reynolds number is roughly proportional to the Reynolds number itself, at least when one is away from singular points of the solution.

Our results are based on some new estimates obtained for the path derivatives, i.e., derivatives with respect to the Reynolds number, of solutions of the Navier-Stokes equations. We have also carried out some computational experiments that support our analytical results. From a practical point of view, our results indicate that it is most efficient to use the simplest type of predictor algorithms within a continuation method. Furthermore, a rather large step in the Reynolds number may be chosen.

Details of the above results may be found in the first item in the bibliography at the end of this section.

b - Parallel algorithms for 3-D flows

We have explored the feasibility of algorithms for three-dimensional flows that can take advantage of parallel processing architectures. Our algorithm involves the choice of a particular form of the governing equations, a finite element discretization, and an advantageous (from a parallel processing point of view) iterative solution strategy for solving the nonlinear system of discrete equations. The computational problem is reduced, for each iteration, to solving an uncoupled system of Poisson equations. Thus we have some obvious coarse-grain parallelism that may be used to advantage on machines (such as the Cray-YMP) that have a few very powerful processors. However, since one must solve Poisson equations, one can also take advantage of any Poisson solvers having fine-grain parallel structure that in turn can make good use of machines with, e.g., hypercube architectures. Among candidate algorithms are conjugate gradient methods and multi-grid methods.

Our own efforts so far have been directed at making sure that the combined modeling, discretization and solution aspects of the numerical algorithm result in practical methods from the points of view of accuracy, stability and efficiency. This was a necessary exercise since many facets of the algorithms we consider are "non-standard" in nature, and in fact, have been subject to considerable debate and dispute in scientific circles. Thus, before declaring the algorithms to be viable in a parallel processing environment, we had to settle some of these outstanding questions.

The algorithm we have studied is a velocity-vorticity based method. For two-dimensional viscous incompressible flow problems, the streamfunction-vorticity formulation is probably the method of choice for use in conjunction with discretization procedures. For three-dimensional flows, the advantages of the streamfunction-vortivity formulation are no so clear cut. Recently, in both engineering and mathematical circles, much interst has been focused on the velocity–vorticity formulation, i.e.,

$$\operatorname{div} \mathbf{u} = 0\,,$$

$$\operatorname{curl} \mathbf{u} = \boldsymbol{\omega}$$

and

$$\nu \operatorname{curl} \operatorname{curl} \boldsymbol{\omega} + \operatorname{curl}(\boldsymbol{\omega} \times \mathbf{u}) = \operatorname{curl} \mathbf{f}\,,$$

where $\mathbf{u}$ and $\boldsymbol{\omega}$ denote to unknown velocity and vorticity fields, respectively, and ν and $\mathbf{f}$ are the given kinematic viscosity coefficient and the body force, respectively. The central problem in using the above formulation is determining boundary conditions for the vorticity at boundaries where the complete velocity field is specified, e.g., at walls. Note that the above equations may be rewritten in the form

$$-\Delta \mathbf{u} = \operatorname{curl} \boldsymbol{\omega}$$

and

$$-\Delta \boldsymbol{\omega} = -\operatorname{curl}(\boldsymbol{\omega} \times \mathbf{u}) + \operatorname{curl} \mathbf{f}\,.$$

We have carried out extensive computational experiments using the velocity-vorticity formulation. Our studies have employed finite element discretizations of three-dimensional problems and have focused on question of accuracy and efficiency, especially in view of different choices of boundary condition treatment. Here we give a brief account of what we have learned.

First, whenever the velocity is given at a boundary, we explicitly use all the information given. Some other researchers choose to only use the normal component of the velocity, leaving the tangential boundary conditions to be implicitly satisfied. Second, for the vorticity, the best thing to do is to require $\boldsymbol{\omega} = \operatorname{curl} \mathbf{u}$ at boundaries where $\mathbf{u}$ is specified. Note that $\boldsymbol{\omega} \cdot \mathbf{n} = \operatorname{curl} \mathbf{u} \cdot \mathbf{n}$ is computable on a boundary where $\mathbf{u}$ is specified; thus, the choice we make is to set the tangential components of the vorticity equal to the tangential components of the curl of the velocity. The latter requires knowledge of interior values of $\mathbf{u}$. We have found, from mathematical, physical and computational points of view, that the above combination of boundary conditions are the prefered ones.

Our next result is concerned with the accuracy of discrete solutions. We have found that in order to achieve the best possible accuracy within a class of interior discretizations, one must approximate the relation $\boldsymbol{\omega} = \operatorname{curl} \mathbf{u}$ to better accuracy on or near the boundary. This may be accomplished by either refining the mesh near the boundary, or by using higher order elements at the boundary. This result, i.e., that one must use better boundary approximations, has not been previously pointed out in either the mathematical or engineering literature.

Our final concern with the velocity-vorticity formulation has been with efficient means of solving the discrete equations. In particular, we have focused on iterative schemes that, within each iteration, uncouple the velocity and vorticity calculations. Of perhaps greatest interest is a scheme that we have found to converge, at least for low values of the Reynolds number, and which requires the solution of six uncoupled Poisson equations at each step of the iteration.

We have completed a paper reporting on the work described above; the paper will appear as an invited chapter in the fourth volume of *Computational Methods in Viscous Flows*; it is the second paper in the references listed at the end of this section.

c - Magnetically coupled flows

We have completed the analysis of finite element approximations of viscous incompressible flows that are affected by magnetic and electric fields. The governing equations are the Navier-Stokes equations and the Maxwell equations, fully coupled so that electromagnetic fields have influence on, and are themselves influenced by, the flow field. Along the way, we had to derive new existence and uniqueness results for these coupled equations. One feature of our work is the incorporation of a variety of (inhomogeneous) boundary conditions into both the mathematical model and into the finite element methods employed. In all cases, we have been able to prove optimal error estimates for the approximate solution.

At the present time we are in the final stages of running computer codes that have been developed. These codes not only illustrate the analytical results that we have derived, but more importantly, have served as a test bed for devising and implementing efficient solution algorithms for the finite dimensional nonlinear system of equations that result from finite element discretizations of the governing system of partial differential equations. We have completed the preparation of a paper that presents the analytical and numerical results described above; this manuscript is the third one in the list of references at the end of this section.

2 - Numerical Approximation of Control Problems

a - Control of viscous incompressible flows

We have completed the analysis of various theoretical and computational issues associated with the control of viscous incompressible flows, specifically those described by the Navier-Stokes equations. All types of controls have been considered. From the point of view of analysis, the easiest cases to treat were distributed controls, e.g., body force controls, and Neumann controls, e.g., stress controls. However, the more interesting case is that of Dirichlet controls, e.g., control by adjusting the velocity at the boundary. The latter has application in, e.g., drag control by blowing or sucking fluid through the boundary. In all cases, one of our aims was to minimize drag by appropriately choosing the control.

Typical of the generality of the problems we have treated is the following situation. We have that the state variables and controls must satisfy the Navier-Stokes system

$$-\nu \operatorname{div}\left((\operatorname{grad}\mathbf{u}) + (\operatorname{grad}\mathbf{u})^T\right) + \mathbf{u}\cdot\operatorname{grad}\mathbf{u} + \operatorname{grad} p = \mathbf{f} + \mathbf{g}_d \quad \text{in } \Omega\,,$$

$$\operatorname{div}\mathbf{u} = 0 \quad \text{in } \Omega\,,$$

$$\mathbf{u} = \mathbf{h}_D + \mathbf{g}_D \quad \text{on } \Gamma_1$$

and

$$-p\mathbf{n} + \nu(\operatorname{grad}\mathbf{u} + \operatorname{grad}\mathbf{u}^T)\cdot\mathbf{n} + \nu\alpha\mathbf{u} = \mathbf{h}_N + \mathbf{g}_N \quad \text{on } \Gamma_2\,.$$

Here Ω is a bounded two or three-dimensional domain and Γ_1 and Γ_2 are parts of its boundary. The state variables are the velocity $\mathbf{u}$ and the pressure p. The functions $\mathbf{f}, \alpha, \mathbf{h}_D$ and $\mathbf{h}_N$ are given. The controls are denoted by $\mathbf{g}_d$ (distributed control), $\mathbf{g}_D$ (Dirichlet control) and $\mathbf{g}_N$ (Neumann control). The controls need not act on all of their respective domains; e.g., $\mathbf{g}_d$ may act on only a subset of Ω and $\mathbf{g}_D$ may act on only a subset of Γ_1. Our optimization problem can involve choosing controls such that either

$$\mathcal{J}(\mathbf{u}) = \frac{1}{2}\int_\Omega |\mathbf{u} - \mathbf{u}_0|^2\, d\Omega$$

or

$$\mathcal{K}(\mathbf{u}) = \frac{\nu}{2}\int_\Omega \left|(\operatorname{grad}\mathbf{u}) + (\operatorname{grad}\mathbf{u})^T\right|^2 d\Omega$$

is minimized. In the first case we want the velocity field to be as "close" as possible to some prescribed field $\mathbf{u}_0$; in the second case we are minimizing the viscous drag.

For the case of Dirichlet controls, we have treated controls that are unknown functions defined on portions of the boundary of the flow region. We have also treated problems where the fluid is allowed to enter or leave the flow region only through a finite number of specified holes on the boundary, and with a specified velocity distribution through the holes. The only control is the amount of fluid that can enter or exit through each hole. This last problem effects considerable simplifications since the set of admissible controls is finite dimensional.

We have fully analyzed questions of existence of optimal controls and of Lagrange multipliers for all cases. We have also developed and analyzed finite element algorithms; all the agorithms we have developed yield optimally accurate approximations. At the present time we are implementing some of these algorithms into a computer code with our main goal being developing efficient solution algorithms for the formidable discrete problem that results from the discretization of the control problem.

This work is been reported in papers 4-7 listed at the end of this section.

b - Boundary controllability problems for the wave equation

We have been trying to develop algorithms for approximately solving controllability problems for the wave equation. Our eventual goal is to extend these algorithms to controllability problems for elastic and viscoelastic structures, including large space structures.

For problems in one space dimensnion, one can easily devise numerous algorithms that can be used to approximately solve controllability problems fo the wave equation. In higher dimensions, the task is not so easy. We believe we have developed and effective means for treating such controllability problems. Consider the model problem

$$\begin{aligned} u_{tt} - \Delta u = 0 &\quad \text{in } (0,T) \times \Omega \\ u(0,\mathbf{x}) = u_0(\mathbf{x}) &\quad \text{for } \mathbf{x} \in \Omega \\ u_t(0,\mathbf{x}) = u_1(\mathbf{x}) &\quad \text{for } \mathbf{x} \in \Omega \\ u(T,\mathbf{x}) = u_2(\mathbf{x}) &\quad \text{for } \mathbf{x} \in \Omega \\ u_t(T,\mathbf{x}) = u_3(\mathbf{x}) &\quad \text{for } \mathbf{x} \in \Omega\,. \end{aligned}$$

Here $u_j, j = 0, \ldots, 3$, are prescribed functions. It is well known that for sufficiently large T there exists boundary controls, either of Neumann or Dirichlet type, such that the above problem has a solution. In fact, in general, the solution is not unique.

Our approach is to solve the above *underdetermined* problem, or rather discrete versions of the above problem, by a least squares techniques. This results in sparse positive definite discrete problems to be solved for which efficient algorithms are known. At the present time we are developing codes that implement these methods with a view towards choosing the best possible among variants of the basic least squares procedure.

A preliminary report describing this work has been completed; it is paper number 8 in the list of references at the end of this section.

3 - Centroidal Voronoi Grids

Voronoi grids and their duals, the Delaunay triangulations, are now in widespread use in the numerical computation of a variety of problems, ranging from partial differential equations to image processing to data compression. These tesselations are simple to define. Given a set of points $\mathbf{z}_j \in \Omega \subset \mathbb{R}^n$, the Vorornoi region for a point $\mathbf{z}_k$ is the set of points in Ω that are closer to $\mathbf{z}_k$ than to any of the other given points. Voronoi regions turn out to be polygons and their usefulness in the numerical solution of partial differential equations stems from the fact that the dual grid is in general a triangulation of the given points $\mathbf{z}_j$ with the property that among all possible triangulations of these points, it is the one with the maximum minimum angle. This, of course, is a desirable property. Furthermore, there has been much research and success recently into developing efficient algorithms for computing Voronoi grids.

In general, the centroids $\mathbf{y}_j$ of the Voronoi polygons need not be anywhere near the points $\mathbf{z}_j$ from which the Voronoi polygons are determined. However, we want to consider the case where $\mathbf{y}_j = \mathbf{z}_j$. More generally, given a region $\Omega \in \mathbf{R}^n$, a positive integer N, and a density function $\rho(\mathbf{x})$, we want to find N points $\mathbf{z}_j, j = 1, \ldots, N$ and N non-overlapping regions $\Omega_j, j = 1, \ldots, N$ covering Ω such that simultaneously each Ω_j is a Voronoi region for $\mathbf{z}_j$, and each $\mathbf{z}_j$ is a centroid, with respect to ρ, of Ω_j. Thus, the set $\{\mathbf{z}_j, \Omega_j\}, j = 1, \ldots, N$, should satisfy

$$|\mathbf{x} - \mathbf{z}_j| < |\mathbf{x} - \mathbf{z}_k| \quad \forall \mathbf{x} \in \Omega_j \text{ and all } k \neq j$$

and

$$\mathbf{z}_i = \frac{\int_{\Omega_j} \mathbf{x}\rho(\mathbf{x})\, d\Omega}{\int_{\Omega_j} \rho(\mathbf{x})\, d\Omega} \quad \text{for } j = 1, \ldots, N\,.$$

We have been able to show that this problem has a (non-unique) solution. Furthermore, we have also considered the following algorithm, known as Lloyd's algorithm in the literature, and shown that it produces a sequence of iterates that converge to a solution. We begin with an arbitratry set of points $\mathbf{z}_j^0 \in \Omega$ that are in general position. At the m-th step, we start with the points $\mathbf{z}_j^{m-1}$ and then compute the Voronoi tesselation of Ω for these points, which we denote by Ω_j^m. This step can be acomplished by well known existing algorithms. We then define $\mathbf{z}_j^m$ to be the center of mass, with respect to the given density function $\rho(\mathbf{x})$, of the region Ω_j^m. We have shown that this algorithm converges in general and have applied it to some practical data compression and image processing problems. We have also studied a variant of the above algorithm wherein the explicit construction of the Voronoi regions is avoided in favor of a stochastic process that yields the same result.

We have also been interested in numerical analysis applications of centroidal Voronoi grids. For example, here is one such application. Consider a function $f(\mathbf{x})$ and its weighted integral over a given region Ω. Now consider piecewise constant type quadrature rules of the type

$$\int_\Omega \rho(\mathbf{x}) f(\mathbf{x})\, d\Omega \approx \sum_{j=1}^{N} \rho(\mathbf{z}_j) f(\mathbf{z}_j) V_j$$

where $\mathbf{z}_j \in \Omega_j$ and $V_j, j = 1, \ldots, N$, are the volumes of the regions Ω_j which tesselate Ω. Then, for the class of Lipschitz continuous functions, among all possible choices of quadrature regions Ω_j and qudarature points $\mathbf{z}_j$, the one that yields the most accurate quadrature rule is one for which the $\mathbf{z}_j's$ and $\Omega_j's$ form a centroidal Voronoi grid. Another application of centroidal Voronoi grids we have examined is to the definition of finite difference schemes on general grids. It turns out that easily defined finite difference schemes that are only first order accurate on arbitrary grids, are second order accurate on centroidal Voronoi grids; since the latter are perfectly useful for tesselating arbitrary domains Ω, we see that centroidal Voronoi grids are useful in generating finite difference schemes on arbitrary domains.

We are currently writing a paper presenting these results; it is paper 9 in the reference list at the end of this section.

4 - A Book on Finite Element Methods for the Navier-Stokes Equations

We have completed the writing of a book on finite element methods for the Navier-Stokes equations. This book is an outgrowth of much of the research we have carried out under AFOSR sponsorship. Thus, it draws form our own considerable expereince, as well as that or others. The goal of the book is to acquaint the interested reader, be it an engineer or mathematician, with the mathematical results and the best algorithms available for solving the Navier-Stokes equations by finite element methods. The book appeared at the end of the summer of 1989; the exact citation is found below at the end of the list of references.

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